VARIATIONAL GAUSSIAN PROCESS FOR OPTIMAL SENSOR PLACEMENT

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Abstract. Sensor placement is an optimisation problem that has recently gained great relevance. In order to achieve accurate online updates of a predictive model, sensors are used to provide observations. When sensors location is optimally selected, the predictive model can greatly reduce its internal errors. A greedy-selection algorithm is used for locating these optimal spatial locations from a numerical embedded space. A novel architecture for solving this big data problem is proposed, relying on a Variational Gaussian Process. The generalisation of the model is further improved via the preconditioning of its inputs: Masked Autoregressive Flows are implemented to learn non-linear, invertible transformations of the conditionally modelled spatial features. Finally, a global optimisation strategy extending the Mutual Information-based optimisation and fine-tuning of the selected optimal location is proposed. The methodology is parallelised to speed-up the computational time, making these tools very fast despite the high complexity associated with both spatial modelling and placement tasks. The model is applied to a real three-dimensional test case considering a room within the Clarence Centre building located in Elephant and Castle, London, UK.

Keywords: Sensor placement, Variational Gaussian Processes, Mutual Information

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1. INTRODUCTION

1

2 Indoor Air Quality (IAQ) impacts health, comfort and quality of life [1], and three
3 basic strategies have been proposed to improve it: control of pollution sources, use
4 of natural/mechanical ventilation, and cleaning of air. In the building context, the
5 management and development of smart monitoring tools can support an adequate

6 IAQ within them (e.g. by automatically opening windows or starting a mechanical
7 air cleaning system). Sensors coupled with indoor pollutant forecasting models can
8 tackle bad IAQ by implementing one of the previously-cited strategies before the
9 indoor pollutant concentration reaches dangerous and adverse levels.

10 In order to achieve accurate, online updates of the predictive model, sensors can
11 be used to provide observations. Spatio-temporal models such as Data Assimilation
12 (DA) provide online learning and forecasting of sensor observations by means of
13 updating the model’s internal view through the incorporation of collected data [2, 3].
14 In this context, sensor positioning has gained relevance [4, 5] as it is crucial to ensure a
15 good quality and usefulness of monitored data. Optimal sensor positioning tools pin-
16 point the discrete spatial locations that possess most conditional information of all
17 other spatial points, thus improving the predictive accuracy of prediction models [6].
18 Hence, sensor placement can be seen as an optimisation problem [4, 5].

19 Early attempts on sensor placement used geometric approaches, supported by the
20 assumption that sensors measure spatial features with a fixed sensing radius [7]. This
21 geometric approach does not take into account the non-linear dynamic behaviour of
22 air motion so, in order to tackle this problem, parametric models [8], non-parametric
23 Gaussian Process (GP) [9] and ensemble Kalman-filters [10] approaches were subse-
24 quently proposed.

25 The main work on this field implements sensor placement using a GP in a 2D space
26 [5]. The time complexity of the placement algorithm is $O(N^4)$, where N denotes the
27 side of the computational domain. The GP is trained on data collected from fixed
28 sensors located in a room, then N is relatively small. The placement algorithm only
29 select the best sensors in the set already provided.

30 In this work, for the first time, a sensor placement model is developed for a 3D
31 domain representing a real case scenario. Also, the model uses temporal sequences
32 of data from fluid dynamic simulations facing then a big data problem. In our
33 case, N is on an scale such that the use of a GP is unfeasible. To address this
34 problem we developed a combination of deep learning, probabilistic frameworks and
35 variational methods, reducing the complexity associated with training, inference and
36 optimisation and thus, enabling us to achieve optimal placement results in a real case
37 scenario. The complexity of our model is, in fact, $O(klM^4)$, where k is the number
38 of sensors, l is the number of iteration needed to optimise the position and M is such
39 that $M \ll N$.

40 The rest of this paper is organized as follows: next section introduces the back-
 41 ground to this work and our main contributions. Section 3 presents the mathemati-
 42 cal formulation of our proposed model, Variational Gaussian Process optimal sensor
 43 placement (VGPosp). Section 4 describes the direct application of VGPosp on a real
 44 indoor environment. The manuscript ends with some conclusions and further work.

45 2. BACKGROUND AND MAIN CONTRIBUTIONS

46 Non-parametric models consist in learning a Gaussian Process (GP) associated with
 47 the phenomenology considered (e.g. pollution levels in indoor environments). In
 48 general, GPs are highly appropriate to study environmental problems as they allow
 49 for learning complex, high-dimensional correlations with uncertainty quantification.
 50 Indeed, non-parametric expressiveness is an advantage over parametric models that
 51 are more prone to the curse of dimensionality [11]. A GP, sometimes referred as
 52 the Bayesian interpretation of neural networks, is fully determined by only two pa-
 53 rameters, namely the mean-function and covariance-function, regardless of their di-
 54 mensionality [12]. Three main GP methodologies can be identified: the Traditional
 55 GP [4, 5], the Sparse GP [13] and the Variational GP [14, 15].

56 Traditional GP is a stochastic process based on prior distribution over functions and
 57 it has been successfully applied for indoor optimal sensor positioning [4, 5]. However,
 58 Traditional GP suffers from the high complexities associated with spatial modelling
 59 $O((mN)^3)$, where N denotes the size of input sensor potential locations and m the
 60 number of physical variables, which explains why the work presented in [4, 5] was
 61 only carried out in two dimensions.

62 Sparse Variational Process (SGP) tackles the inconvenient $O((mN)^3)$ computational
 63 complexity associated with Traditional GP [16]. This method constructs an approx-
 64 imation based on a small subset of size $\hat{N}$, namely inducing points. This optimisa-
 65 tion results in a reduced complexity $O((mN)\hat{N}^2)$, enabling the scalability of training
 66 data-points from the previous limit of a few thousand to the range of millions [17].
 67 In general, sparsity can be achieved by working on a low-rank representation of the
 68 full kernel [18]. The key idea is to approximate the prior or modify the likelihood
 69 function, thus creating a model selection problem solving the optimisation for the
 70 approximation of the truth [13]. However, the main criticism to SGPs is that they
 71 learn unknown hyperparameters, potentially leading them to underestimate variance
 72 and thus over-fitting [14, 15].

73 Alternatively, Variational Gaussian Process (VGP), a variational method for SGP,
 74 was developed [14, 15] to deal with the approximation of model components that

are hard to compute. Inducing points are variational parameters selected by minimising the Kullback-Leibler (KL) divergence [14, 15]. The kernel hyperparameters and inducing points are jointly optimised by maximising a lower bound (Evidence Lower BOund (ELBO)) of variational distribution over the functions latent values [14, 15, 19]. The key innovation, is that the likelihood and the GP prior are not modified, separating the model and the inference. The variational posterior iteratively approaches the true posterior.

The datasets used to train a GP usually comprises data coming from monitoring sensors during extensive field experiment periods. This training dataset usually suffer from being non-Gaussian distributed, rendering it unusable for GP learning [20]. In this regards, several methodologies to precondition, normalise and render the training dataset Gaussian can be mentioned: Variational Autoencoder [21], Autoregressive Flows [22], Normalising Flows [23], Masked Autoencoder for Distribution Estimation (MADE) [24], and Masked Autoregressive Flows (MAF) [20]. The MAF approach is a stack of MADE networks [24, 20] and has proved its competitiveness over the other methodologies in terms of accuracy [20].

Even if VGP can deal with non-Gaussian distributed data, the preconditioning phase of learning non-linear, invertible transformations between the conditional input distributions and output Gaussian family of distributions enables greater generalisation of the learned spatial model.

At this stage, the actual sensors placement problem can then be addressed using the trained GP. Indeed, the placement algorithm is solved in an embedded space that is predicted by a GP [14, 15]. In other words, the GP serves as a numerical setting for the optimisation problem: conditional predictions are used to generate the covariance matrix taken as input by the placement algorithm. The complexity associated with the placement task is $O(N^4)$, where N denotes the size of input sensor potential locations.

Mutual Information (MI) [4, 5] and minimum cross entropy [25, 26] are some of the metrics traditionally used. The use of minimum cross entropy tends to maximise the distance between sensors. In indoor environment problems, this results in having sensors located near the boundary of the domain, i.e. near the walls, thus loosing information monitored [26, 5]. On the other hand, information gain or Mutual Information [4] shifts the amount of information captured by a single random variable to the information each random variable has of the other unobserved one. More specifically, considering a finite set of possible placement locations, by maximising the objective metric, it evaluates how well a given smaller subset of sensor locations describes the values of the unselected other locations. This paper considers the

112 optimisation problem of sensor placement in indoor environments by separating the
 113 problem into the learning of a spatial model, i.e. Gaussian Process training, and
 114 the optimisation algorithm itself, i.e. optimal sensor placement. It is demonstrated
 115 that with a combination of deep learning, probabilistic frameworks and variational
 116 methods, the complexity associated with training, inference and optimisation can be
 117 significantly reduced in order to achieve optimal placement results. This paper builds
 118 on existing 2D sensor placement algorithm [4, 5] and the latest VGP spatial modelling
 119 technologies [14, 15]. Its value is found primarily in the pairing of technologies that
 120 in turn improve the existing methods of sensor placement.

121 The choice of the technologies used in this work are detailed and argued in the
 122 following points:

- 123 • **Preprocessing input distribution** A Masked Autoregressive Flow (MAF)
 124 is used to normalise the training dataset suffering from being non-Gaussian
 125 distributed [20] making our methodology greatly generalised as well as im-
 126 proving the accuracy.

- 127 • **Spatial model** A major challenge facing scalable sensor placement is over-
 128 come by deploying a Variational Gaussian Process (VGP), using a low
 129 rank approximation that is far more scalable and also addresses the ques-
 130 tion of model generalisation. In particular, this helps to tackle the limit-
 131 ing $O((mN)^3)$, high polynomial time complexities associated with GPs to
 132 $O((mN)\hat{N}^2)$ where $\hat{N}$ denotes the number of approximate posterior samples
 133 computed in the VGP. Using a VGP is a good trade-off between efficiency
 134 and accuracy [14, 15].

- 135 • **Sensor placement algorithm** The Mutual Information (MI) based place-
 136 ment algorithm [4, 5] is extended with a Markov-Chain Monte Carlo (MCMC)
 137 wrapper to fine-tune the sensor placement and tackle the time complexity
 138 $O(N^4)$ and achieve $O(klM^4)$, where k is the number of sensors, l is the num-
 139 ber of iteration needed to optimise the position and M is such that $M \ll N$.
 140 The use of MCMC leads to similar placement results in a fraction of the
 141 computation time required when not using it. Error propagation through
 142 the system does exist due to this approximation, however, it is shown in the
 143 paper to be a worthwhile trade-off.

144 The technologies used in this paper are general and are not limited to the test case
 145 of sensor placement in indoor environments, even though their integrated implemen-
 146 tation was designed accordingly. In fact, the core underlying technology used in the

spatial model, i.e. Variational Gaussian Process, has been successfully deployed for a multitude of other domains ranging from kriging to robotics [27].

In addition to the new pairing of technologies proposed in this paper, the novelties of this work also lie in:

- **The simulated training data** In order to achieve scalable and reduced cost deployment of sensor placement optimisation, simulation data was used for model training, replacing the expensive option of collecting large amounts measurements from installed sensors. As an example, the training dataset used in [5] consists of 52 sensors, located on a 2D plan. In this paper, the simulated training dataset is much larger, i.e. more reliable, and consist of 10,000 sensor locations distributed in 3D.
- **The increase in dimensionality** This paper increases the dimensionality of the learning problem in order to capture further correlations between hidden features as well as the output features, resulting in 3-dimensional spatial placement. The 3D placement made it possible for the model to capture more realistic and complex physical phenomena such as thermal stratification for example.
- **The fine-tuning of sensor placement** The MCMC wrapper algorithm is used to increase the overall Mutual Information captured. The base set of potential sensor location is fine-tuned to include other regions in the continuous space having higher MI. This means the selection pipeline is a more optimal set of possible placement coordinates to choose from. Additionally, the implementation is easy to be customised and makes our methodology generalisable.
- **The fully parallel and scalable implementation** The methodology presented in this paper is done through a multi-threaded parallel implementation. The computational graph based implementation, using the TensorFlow library [28], greatly speeds up the computational times.

3. THE VARIATIONAL GAUSSIAN PROCESS FOR OPTIMAL SENSOR PLACEMENT (VGPOSP) MODEL

This section introduces the theoretical concepts and mathematical formulation that were developed and implemented as part of the proposed model architecture.

Let X be the solution of a dynamic system:

$$(3.1) \quad \dot{X} = F(X, t)$$

180 where, t denotes the time and $X = [X_1, \dots, X_m]$ denotes a vector of m state vari-
 181 ables¹ such that $X_i \in \mathbb{R}^N$, $\forall i = 1, \dots, m$. In the following, $X_t = X(t)$ denotes the
 182 solution of the dynamic system at time t and $X_{i,t} = X_i(t)$ the i -th state variable at
 183 time t .

184 Given a temporal sequence $X_{t_1}, \dots, X_{t_n}$ of n solutions of the dynamical system de-
 185 fined in equation (3.1), with $X_{t_i} = [X_{1,t_i}, \dots, X_{m,t_i}] \forall i = 1, \dots, n$, the Variational
 186 Gaussian Process for optimal sensor placement (VGPosp) model consists of the fol-
 187 lowing main steps described in the sub-sections 3.1 to 3.3.

- 188 • **Section 3.1 - Preprocessing and preconditioning**
 - 189 – Preconditioning of input vector distributions using Masked Autoregres-
 190 sive Flows (MAF).
 - 191 – Convert time-series to vector value distributions at distinct spatial re-
 192 gions.
- 193 • **Section 3.2 - Variational Gaussian Process**
 - 194 – Sampling algorithm, input vectors spatial training.
 - 195 – Variational Gaussian Process (VGP) training.
- 196 • **Section 3.3 - Placement algorithm**
 - 197 – Selection of a set S of considered input coordinates.
 - 198 – Generate target vectors with VGP inference at coordinates.
 - 199 – Covariance matrix of values indexed by set S .
 - 200 – Greedy selection algorithm of coordinates with maximal Mutual Infor-
 201 mation (MI).
 - 202 – Markov-Chain Monte Carlo (MCMC) based fine-tuning of coordinates.

203 **3.1. Pre-processing and preconditioning.** The temporal sequence $X_{t_1}, \dots, X_{t_n}$
 204 requires a pre-processing to be suitable for the spatial model and the inference step
 205 during the placement algorithm. The pre-processing consists of the following steps,
 206 also described in Figure 1:

- 207 (1) X is first normalised to a mean value of 0 and standardised to achieve a
 208 standard deviation of each feature of 1.

¹For example, as shown in Section 4, for fluid dynamic simulations in indoor environment, $X = [T, P, C]$, where T is the temperature, P the pressure and C the pollutant concentration.

209 (2) Secondly, a Masked Autoregressive Flow (MAF) is implemented to learn
 210 invertible, non-linear transformations between the non-Gaussian distributed
 211 features and the target Gaussian family of distributions.

FIGURE 1. Pre-processing and pre-conditioning steps.

212 Firstly, the mean of the temporal sequence for each state variable X_i , $i = 1, \dots, m$,
 213 is computed, i.e. the vector

$$(3.2) \quad \bar{X} = [\bar{X}_1, \dots, \bar{X}_m]$$

214 where

$$(3.3) \quad \bar{X}_i = \frac{\sum_{j=1}^n X_{i,t_j}}{n}, \quad \forall i = 1, \dots, m$$

215 The vector $\bar{X}$ in equation (3.2) is used to train the Masked Autoregressive Flows
 216 (MAF) in order to make our input variables Gaussian distributed. MAF is a neural
 217 network that executes a normalising flow non-linear transformation at each neuron.
 218 MAF can be also computed as a stack of autoregressive Masked Autoencoder for
 219 Distribution Estimation (MADE) networks [20, 24] where each model uses the vector
 220 $\bar{X}$ in equation (3.2). The Autoregressive property of MAF defined from time-series
 221 analysis, predicts a future value of a variable from a linear combination of its past
 222 values. Each MADE learns the distribution of the state variables.

223 The MAF model can be defined as follows [22]:

$$(3.4) \quad \bar{X}_N = f_N(\bar{X}_{N-1}, \bar{X}_{N-2}, \dots, \bar{X}_1)$$

224 where f_N has a polynomial form such that [20]:

$$(3.5) \quad \bar{X}_N = \theta_0 + \theta_1 \bar{X}_{N-1} + \theta_2 \bar{X}_{N-2} + \dots + \theta_p \bar{X}_{N-p}$$

225 where θ_i are the polynomial coefficients.

226 Normalising flows apply a sequence of N invertible, differentiable transformation
 227 functions f_N in $p(\bar{X})$. A base distribution $p(\bar{X}')$ is specified most likely from the
 228 family of Gaussian distributions [20], where p denotes the probability distribution.
 229 The procedure begins with this initial distribution $p(\bar{X}')$ [23].

$$(3.6) \quad p(\bar{X}) = p(\bar{X}') \left| \det \frac{\partial f^{-1}}{\partial \bar{X}'} \right|$$

230 A chain rule can then be applied to the conditionals of a joint distribution.

$$(3.7) \quad p(\bar{X}) = \prod_{i=1}^N p(\bar{X}_i | \bar{X}_{i-1}, \bar{X}_{i-2}, \dots, \bar{X}_1) = \prod_{i=1}^N p(\bar{X}_i | \bar{X}_{<i})$$

231 After each non-linear transformation the distribution becomes more complex. Sam-
 232 pling from this transformed distribution is done via the flow of a straightforward
 233 sample from the original $p(\bar{X})$ Gaussian distribution through the non-linear trans-
 234 formations. The entropy of the resultant distribution is computed with the logarithm
 235 of the transformations:

$$(3.8) \quad \log p(\bar{X}_N) = \log p(\bar{X}_0) - \sum_{i=1}^N \ln \left| \det \frac{\partial f_N}{\partial \bar{X}_{i-1}} \right|$$

236

$$(3.9) \quad p(Y) = \prod_{i=1}^N \left(f_N^{-1}(Y) \right) \left| \det \frac{\partial f_N^{-1}}{\partial Y} \right|$$

237 The vector

$$(3.10) \quad Y = [Y_1, \dots, Y_m] \in \mathbb{R}^{m \times N}, \quad \text{with } Y_j \in \mathbb{R}^N \quad \forall j = 1, \dots, m$$

238 is the set of normalised state variables which are input of the Variational Gaussian
 239 Process introduced in next section.

240 **3.2. VGP training and inference.** Given the data set $\{Y_j\}_{j=1}^m$ of $Y_j \in \mathbb{R}^N$ as
 241 defined in equation (3.10), the m source-target pairs $\mathcal{D} = \{(Y_j, T)\}_{j=1}^m$, where T is a
 242 target² [29]. We aim to learn a function over all source-target pairs:

$$(3.11) \quad T = g(Y_j)$$

²In some application, $T = Y_j$ for a fixed j can be assumed.

243 where $g : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is unknown. Let the function g decouple as $g = (g_1, \dots, g_N)$,
 244 where each $g_i : \mathbb{R}^N \rightarrow \mathbb{R}$. A GP regression [12] estimates the functional form of g by
 245 placing a prior,

$$(3.12) \quad p(g) = \prod_{i=1}^N \mathcal{GP}(g_i; 0, \Sigma_{ij}),$$

246 where Σ_{ij} denotes a covariance evaluated over pairs of inputs $Y_i Y_j \in \mathbb{R}^N$ [12]:

$$(3.13) \quad \Sigma_{ij} = \frac{\sum_k Y_{ik} Y_{jk}^T}{N}$$

247 A variational Gaussian process (VGP) is a Bayesian non-parametric variational
 248 model that admits arbitrary structures to match posterior distributions. As de-
 249 scribed in the following steps, the VGP generates approximate posterior samples Z
 250 by generating latent inputs, warping them with random non-linear mappings, and
 251 using the warped inputs as parameters to a mean-field distribution. The random
 252 mappings are drawn conditional on variational parameters. The VGP specifies a
 253 generative process for posterior latent variables Z . At the first step it draws la-
 254 tent input $\xi \in \mathbb{R}^N : \xi \sim \mathcal{N}(0, I)$ and a non-linear mapping $g : \mathbb{R}^N \rightarrow \mathbb{R}^N$ condi-
 255 tioned on $\mathcal{D} : g \sim \prod_{i=1}^N \mathcal{GP}(0, \Sigma_{\xi\xi}) | \mathcal{D}$. Then it draws approximate posterior samples
 256 $Z \in \text{supp}(p) : Z = (Z_1, \dots, Z_{\hat{N}}) \sim \prod_{i=1}^{\hat{N}} q(g_i(\xi))$. Marginalising over all latent inputs
 257 and non-linear mappings, the VGP is [29]:

$$(3.14) \quad q_{VGP}(Z; \theta, \mathcal{D}) = \iint \left[\prod_{i=1}^{\hat{N}} q(Z_i | g_i(\xi)) \right] \left[\prod_{i=1}^{\hat{N}} \mathcal{GP}(g_i; 0, \Sigma_{\xi\xi}) | \mathcal{D} \right] \mathcal{N}(\xi; 0, I) d\xi d\xi.$$

258 The VGP is parametrised by kernel hyperparameters θ and variational data [29, 12].
 259 The random function interpolates the values in the variational data, which are opti-
 260 mised to minimise the Kullback–Leibler divergence [30]. It defines a measure between
 261 two probability density functions: $q_{VGP}(Z; \theta, \mathcal{D})$ and $q^*(Z|Y)$, where $q^*(Z|Y)$ is the
 262 posterior distribution [31].

$$(3.15) \quad D_{KL}(q_{VGP}(Z; \theta, \mathcal{D}) || q^*(Z|Y)) = \mathbb{E}_q \left[\log \frac{q_{VGP}(Z; \theta, \mathcal{D})}{q^*(Z|Y)} \right]$$

$$= \mathbb{E}_q \left[\log q_{VGP}(Z; \theta, \mathcal{D}) - \log q^*(Z|Y) \right]$$

263 where [19] $\mathbb{E}[f(x, \theta)] = \int_{\theta} f(x, \theta) d\theta$, where f denotes a distribution function. An
 264 approximating distribution is chosen from a predefined family of distributions with

parameters: θ .

$$(3.16) \quad q_\theta(Z|Y) = \operatorname{argmin}_\theta D_{KL}\left(q_{VGP}(Z; \theta, \mathcal{D}) || q^*(Z|Y)\right)$$

When the KL-divergence converges to 0 (see the Theorem of the Universal approximation in [29]), the posterior is approximately the same as the learned posterior. Minimising KL-divergence is done via the objective function, defined by the Evidence Lower Bound (ELBO), parameterised by the parameters θ . The maximisation of this function is equivalent as minimising KL with a difference measured by a constant factor [23]. The objective is summed over all data-points [19]:

$$(3.17) \quad \text{ELBO}(\theta) = \sum_{i=1}^{\hat{N}} \mathbb{E}_{q_\theta(Z|X_i)} [\log q_{VGP}(Z; \theta, Y_i) - \log q_\theta(Z|Y_i)]$$

When applied to the marginal probability of the evidence [29, 15], the objective lower bound on the marginal likelihood can be quantified by the ELBO:

$$(3.18) \quad \text{ELBO}(\theta) = \mathbb{E}_q[\log q_{VGP}(Z; \theta, X)] - \mathbb{E}_q[\log q_\theta(z|x)]$$

Posterior is therefore the sum of the ELBO and the KL term:

$$(3.19) \quad \log q(Z) = \text{ELBO}(\theta) + D_{KL}(q_\theta(Z|Y) || q^*(Z|Y)).$$

An approximate solution in the mean-field [32] is sought to learn parameters of the marginal likelihood [33], obtaining an approximate posterior distribution of the true posterior. The mean-field approximation of variational inference allowed for the approximate $q_\theta(Z|Y)$ distribution to be considered as a factor of $\hat{N}$ independent latent variable partitions $q_\theta(Z|Y_i)$.

$$(3.20) \quad q^*(Z|Y) \approx q_\theta(Z|Y) = \prod_{i=1}^{\hat{N}} q_\theta(Z|Y_i)$$

then it yields $g \sim q^*(Z|Y)$ [34].

3.3. Placement Algorithm. In this section, the Placement algorithm of VGPosp model is introduced. The algorithm computes optimal coordinates for sensor placement following three main steps as described in Figure 2 and detailed in Algorithm 1.

The set of coordinates $\mathcal{V}$ initially consists of N grid point: $|\mathcal{V}| = N$. Our placement algorithm is mainly based on the Mutual Information (MI) based placement algorithm [4, 5] which is extended in this paper with a MCMC wrapper to fine-tune

FIGURE 2. Graphical representation of the main steps of the Variational Gaussian Process for optimal sensor placement (VGPosp) model

the sensor placement and tackle the time complexity $O(N^4)$ and achieve $O(klM^4)$, where k is the number of sensors, l is the number of iteration needed to optimise the position and M is a predefined small subset of N such that $M \ll N$. In fact, the first step of Algorithm 1 consists of identifying all the possible locations which constitutes a set S , $|S| = M$ (see points 1 and 2 in Figure 2). The set S is an input of Algorithm 1. Other inputs are the number k of sensors to place and the number l of maximum iterations for the optimisation process. We implement an optimisation method to identify a set $\mathcal{A}$ as the placement output from the predefined set S of input coordinates [4] such that $|\mathcal{A}| = k$. The second step of Algorithm 1 consists in sampling m state variables from value distributions in Y at corresponding spatial regions/cells (see point 3 in Figure 2). For each state variable in Y (see point 4 in Figure 2), the samples T are produced by the function g which is computed by a

Algorithm 1: The Variational Gaussian Process for optimal sensor placement (VGPosp) algorithm.

Input: number of sensors: k , space of coordinates: S , maximum number of iterations: l ; ϵ

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1  $\mathcal{A}^* = \emptyset$                                  $\triangleright$  initialise the set of optimal sensors locations
2  $\Sigma = \emptyset$                                  $\triangleright$  initialise the covariance matrix
3  $\delta_{\bar{y}} = 0$                                  $\triangleright$  initialise the mutual information parameter
4 while  $ii < k$  do
5   while  $it < l$  do                                 $\triangleright$  compute the covariance matrix
6   for  $i \in S$  do
7     for  $t_k \in [t_0, t_n]$  do
8        $T_{ik} = g(Y_{ik})$                                  $\triangleright$  VGP function in 3.11
9        $T_i = [T_{i0}, T_{i1}, \dots, T_{in}]$ 
10    for  $j \in S$  do
11      for  $t_k \in [t_0, t_n]$  do
12         $T_{jk} = g(Y_{jk})$                                  $\triangleright$  VGP function in 3.11
13         $T_j = [T_{j0}, T_{j1}, \dots, T_{jn}]$ 
14      compute  $\Sigma_{ij}$                                  $\triangleright$  using equation (3.13)
15     $\mathcal{A}, \delta_{i^*} \leftarrow \text{Algorithm 2}(\Sigma, S, k)$      $\triangleright$  estimate the mutual information
16    if  $\delta_{i^*} > \delta_{\bar{i}}$  or  $\mathcal{A}^* = \emptyset$  then
17       $\mathcal{A}^* = \mathcal{A}$ 
18       $\delta_{\bar{i}} = \delta_{i^*}$ 
19     $it++$ 
20   $ii++$ 
21 return  $\mathcal{A}^*$ 

```

VGP as described in section 3.2 (see points 9-14 in Algorithm 1):

$$\forall j \in S, \quad T_{jk} = g(Y_{jk}), \quad T_j = [T_{j0}, T_{j1}, \dots, T_{jn}]$$

284 Then the covariance matrix of the values T_j are computed for the locations specified
285 in S using equation (3.13) (see points 5 and 6 in Figure 2). We also define the
286 covariance matrices related to a subset $\mathcal{A}$ such that:

$$(3.21) \quad \Sigma_{i\mathcal{A}} = \begin{bmatrix} \Sigma_{i1} & 0 & 0 & \dots \\ 0 & \Sigma_{i2} & 0 & \dots \\ \vdots & \ddots & \ddots & \vdots \\ \dots & 0 & 0 & \Sigma_{ik} \end{bmatrix}$$

287 where Σ_{ij} is defined in equation (3.13) and $k = |\mathcal{A}|$. $\Sigma_{i\mathcal{A}}$ is used in the final step of
 288 Algorithm 1 which maximise the mutual information (see points 7 and 8 in Figure 2),
 289 as described in Algorithm 2, where H is the conditional entropy function defined as
 290 (see [5]):

$$(3.22) \quad H(i|\mathcal{A}) = \frac{1}{2} \log \Sigma_{i\mathcal{A}}^2 + \frac{1}{2} (\log(2\pi) + 1)$$

291 and where δ_i denotes the mutual information parameter [5]:

$$(3.23) \quad \delta_i = \frac{\Sigma_{ii}^2 - \Sigma_{i\mathcal{A}} \Sigma_{\mathcal{A}\mathcal{A}}^{-1} \Sigma_{\mathcal{A}i}}{\Sigma_{ii}^2 - \Sigma_{i\bar{\mathcal{A}}} \Sigma_{\bar{\mathcal{A}}\bar{\mathcal{A}}}^{-1} \Sigma_{\bar{\mathcal{A}}i}}$$

Algorithm 2: Maximise Mutual Information (MI) using lazy evaluations.

Input: Covariance matrix Σ_{ij} , number of sensors k , set of coordinates $\mathcal{S}$

```

1  $\mathcal{A} \leftarrow \emptyset$ 
2 foreach  $i \in \mathcal{S}$  do
3    $\delta_i \leftarrow +\infty$ 
4 for  $j=1$  to  $k$  do
5   foreach  $i \in \bar{\mathcal{A}} = \mathcal{S} \setminus \mathcal{A}$  do
6      $current_i \leftarrow false$ 
7   while  $current_i == true$  do
8      $i^* \leftarrow \operatorname{argmax}_{i \in \mathcal{S} \setminus \mathcal{A}} \delta_i$ 
9     if  $current_{i^*} == true$  then
10       break
11       Compute  $\Sigma_{i\mathcal{A}}$  ▷ using equation (3.21) for  $i$  and  $\mathcal{A}$ 
12       Compute  $\Sigma_{i\bar{\mathcal{A}}}$  ▷ using equation (3.21) for  $i$  and  $\bar{\mathcal{A}}$ 
13        $\delta_{i^*} \leftarrow H(i|\mathcal{A}) - H(i|\bar{\mathcal{A}})$  ▷ with  $H$  defined in (3.22)
14        $current_{i^*} \leftarrow true$ 
15    $\mathcal{A} \leftarrow \mathcal{A} \cup i^*$ 
16 return  $\mathcal{A}$ 

```

292 We developed a MCMC based wrapper that works with a smaller grid of points
 293 $\mathcal{S}$, then identifies the vertices of the grid $\mathcal{A}$ that are potential frontiers to be ex-
 294 plored further. These optimal coordinates in $\mathcal{S}$ are thus adjusted. If the adjustment
 295 has improved the overall mutual information we keep the modification. Using this
 296 technique we iteratively adjust $\mathcal{S}$ until the mutual information value converges.

3.4. **Implementation.** A code implementing Algorithm 1 and Algorithm 2 using TensorFlow 1.4 [28] is available at <https://github.com/roxarcucci/VGPosp.git>. Instructions for running the tests and algorithms are described in the file README.md. The algorithms were initially implemented in Python and reimplemented later in TensorFlow in order to further improve the efficiency of the run-time through multi-threaded, parallelised execution and automatic scalability to more computational cores. Our implemented model is represented in the form of a computational data-flow graph that is instantiated once a session object is defined. The built-in TensorFlow compiler identifies all dependencies within our algorithms and assigns multi-threaded computational tasks to our resources. TensorBoard creates a visual representation of the nodes and connections, it enables the developer to debug connectivity errors. The Scalars tool that allows the tracking of any metric of interest during model training or optimisation was also used.

4. RESULTS AND DISCUSSIONS

In this section, two test cases are used to discuss our Variation Gaussian Process for optimal sensor placement (VGPOsp):

- The first test case, named the sine model, is a simplified two-dimensional model of a sine function to test the efficiency, accuracy and precision of VGP compared to GP. The comparison between GP and VGP is done only for the sine model as the complexity of GP is too high to be trained for a real test case.
- The second test case is a real three-dimensional test case considering a room within the Clarence Centre building located in Elephant and Castle, London, UK. In this test case, the predictive model is the Computational Fluid Dynamics (CFD) software Fluidity. Optimal sensors location is proposed. The benefit of using sensors optimally located is proved by showing how the predictive model error can be more efficiently reduced by using Data Assimilation technology.

4.1. Test case 1: Sine model. This section aims to compare the efficiency, the accuracy and the precision of GP and VGP. The test sine function used is defined in equation(4.1).

$$(4.1) \quad f(x, y) = \sin\left(\frac{2}{3}\pi x\right) + \sin\left(\frac{2}{3}\pi y\right)$$

In order to prove that VGP is more efficient than a GP approach, the training time as a function of the number of training points for both method are shown in Figure 3.

FIGURE 3. Training time as a function of number of training points when using a Gaussian Process (GP) or a Variation Gaussian Process (VGP).

Up to 150 number of training points, the GP and the VGP method both take a little bit less than 10 sec to be trained. However, when using more training points, i.e. more than 150 number of points, the training time of the GP increases drastically, while the VGP training time stays constant, around 10 sec, independently of the number of points. For example, when considering 600 training points, the training time is divided by 5.5 when using the VGP approach.

The accuracy e and the root mean squared error (also called precision), $RMSE$ of the model $\mathcal{M}$ are:

$$(4.2) \quad e_{\mathcal{M}}(N) = \sum_{i=1}^N |f_{True}(x_i, y_i) - f_{\mathcal{M}}(x_i, y_i)|$$

where N is the number of training points, and

$$(4.3) \quad RMSE_{\mathcal{M}}(N) = \sqrt{\frac{\|F_{\mathcal{M}} - F_{True}\|_{L^2}}{\|F_{True}\|_{L^2}}}$$

where $F_{\mathcal{M}}$ and F_{True} denote the vectors $F_{\mathcal{M}} = [f_{\mathcal{M}}(x_1, y_1), \dots, f_{\mathcal{M}}(x_N, y_N)]$ and $F_{True} = [f_{True}(x_1, y_1), \dots, f_{True}(x_N, y_N)]$, the *True* model denotes the function in equation (4.1) and the model $\mathcal{M}$ stands for GP or VGP.

The accuracy (equation (4.2)) and the precision (equation (4.3)) of the two models as a function of the number of training points are shown in Figure 4. From Figure 4a, when using less than 150 training points, the two models highlight the worst accuracy, i.e. the highest values. When using more than 150 number of training points, it can be seen that the accuracy of GP is lower than 0.03, while the VGP accuracy is lower

FIGURE 4. (A) Accuracy e and (B) Precision $RMSE$ as a function of number of training points when using a Gaussian Process (GP) and a Variation Gaussian Process (VGP).

than 0.02. Globally, the VGP method is slightly more accurate than GP even if the accuracy can be considered as the same order of magnitude. However, looking at Figure 4b, the GP model is more precise than the VGP. For both model, the RMSE is relatively high when using less than 200 number of training points. When using more training points, the RMSE reaches a plateau with values for the GP and VGP model of about 0.12 and 0.17, respectively.

Overall, it has been shown that the VGP method is a good trade-off between the efficiency, the accuracy and the precision and will then be used as such an assumed tool in the second test case.

4.2. Test case 2: Real test case.

4.2.1. *Predictive model: Computational Fluid Dynamics simulation using Fluidity software.* The simulated data used to train our VGPosp is obtained using Fluidity, a parallel open-source CFD software (<http://fluidityproject.github.io/>). It uses finite elements to solve the following incompressible three dimensional Navier-Stokes equations, continuity equation (4.4) and momentum equation (4.5), on unstructured grids [35]:

$$(4.4) \quad \nabla \cdot \bar{u} = 0$$

$$(4.5) \quad \frac{\partial \bar{u}}{\partial t} + \bar{u} \cdot \nabla \bar{u} = -\frac{1}{\rho} \nabla \bar{p} + \nabla \cdot [(\nu + \nu_\tau) \nabla \bar{u}]$$

where $\bar{u}$ is the resolved velocity (m/s), $\bar{p}$ is the resolved pressure (Pa), ρ is the fluid density (kg/m³), ν is the kinematic viscosity (m²/s) and ν_τ is the anisotropic eddy

viscosity (m^2/s).
Turbulence is resolved using Large Eddy Simulation (LES), where the eddies smaller than a scale Δ are parametrised using a subgrid-scale module, while the larger eddies are fully resolved. The subgrid-scale model in Fluidity is based on the Smagorinsky model [36, 37].

The transport of a scalar field C (i.e, a passive tracer or pollutant concentration) in kg/m^3 is expressed using the advection-diffusion equation (4.6):

$$(4.6) \quad \frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C) = \nabla \cdot (\overline{\kappa_C} \nabla C) + F$$

where $\mathbf{u}$ is the velocity vector (m/s), $\overline{\kappa_C}$ is the diffusivity tensor of the pollutant in an excess of air (m^2/s) and F represents the source terms ($\text{kg}/\text{m}^3/\text{s}$).
The temperature field T (Kelvin) is expressed using equation (4.7):

$$(4.7) \quad \frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u}T) = \nabla \cdot (\overline{\kappa_T} \nabla T) + \frac{Q}{\rho c_p}$$

where $\mathbf{u}$ is the velocity vector (m/s), $\overline{\kappa_T}$ is the thermal diffusivity tensor (m^2/s), Q represents thermal source terms (W/m^3), ρ is the fluid density (kg/m^3) and c_p is the fluid specific heat capacity ($\text{J}/\text{kg}/\text{K}$). The behaviour of the atmospheric boundary layer in Fluidity is represented using a turbulent inlet velocity based on a synthetic eddy method [38, 39]. Fluidity uses mesh adaptivity where the mesh can be dynamically refined, during the simulation, in areas of physical significance to the user [40].

4.2.2. Test case set up description. The test case considered in this paper is a room within the Clarence Centre building located at London South Bank University (LSBU) near Elephant and Castle in London, UK (Figure 5). The test room has three windows depicting in blue in Figure 5. This test site was used to conduct a one-day field study in January 2018 with the MAGIC project (<http://www.magic-air.uk/>, [41]) during which 7 sensors were monitoring the indoor temperature and CO_2 concentration. The CFD simulation performed in this paper aims to replicate a cross ventilation scenario, where the test room windows on both sides of the building were opened.

As shown in Figure 6, the computational domain considered to do the numerical simulations includes the entire Clarence building and the test room, as well as the immediate building upwind in order to replicate the local flow conditions near the windows. The mesh is defined such that the resolution is increased in the room (setting the grid edge length to 0.1 m) and particularly at the openings (grid edge length set to 0.02 m). It progressively decreases in the overall domain to reach an

FIGURE 5. The test case room is located in Clarence Centre building in London, UK. The red dots denotes the location of sensors during a field experiment and blue rectangles shows the location of the three windows.

FIGURE 6. Computational domain and surface mesh of the area of interest showing the Clarence Centre and the upwind building as well as the test case room. The blue arrows denote the wind direction.

edge length of 10 m away from the room as shown in Figure 6, which gives an overall number of 285,700 cells, i.e. grid points, in the mesh. The total number of nodes within the room is about 1.5×10^5 .

The boundary conditions are set to replicate the experimental conditions. A log-law turbulent inlet velocity is imposed upwind, corresponding to a wind direction of 201° . It is parametrised with an incoming wind velocity of 2.58 m/s at 28.5 m. No slip

FIGURE 7. Concentration field of CO_2 on two vertical slices in the room at different time. The scale is between $7.2 \times 10^{-4} kg/m^3$ (blue colour) and $2.58 \times 10^{-3} kg/m^3$ (red colour).

boundary conditions are imposed at the bottom of the domain and on the walls of the test room. The initial temperature is set to 19.5 °C inside the room and 9.1 °C outside. Before opening the windows, based on sensors data, the average CO_2 concentration in the room is set to $2.58 \times 10^{-3} kg/m^3$ (1420 ppm) while $7.2 \times 10^{-4} kg/m^3$ (400 ppm), is prescribed outside as a background pollution level.

The simulation was run in parallel on 20 CPU and for an overall simulation time of 15 min, leading to about 3500 timesteps. In this paper, the target variables is the concentration C of CO_2 within the room. As an example, the evolution of the concentration field on different planes in the room within the room at different times are shown in Figure 7 and Figure 8. At the beginning of the simulation, the outdoor air enters the room gradually and concentration stratification starts to occur after 2 minutes 30 seconds. It can be seen that the concentration in the room starts to reach a steady state after 5 minutes and does not change anymore after 15 minutes of simulations.

4.2.3. Results. The training set consists in 10,000 points, exceeding the amount used in previous work by a factor of 150 [4, 5]. The quantity and 3D spatial positioning of

FIGURE 8. Concentration field of CO_2 on an horizontal plane in the room at different time. The scale is between $7.2 \times 10^{-4} kg/m^3$ (blue colour) and $2.58 \times 10^{-3} kg/m^3$ (red colour).

the training set was sufficient to capture the phenomenology of the indoor environment. The CFD results used to train the VGP are taken between 2 min 30 sec and 5 min, period during which the stratification of the concentration is established. The solution of this dynamical system X in (3.1) includes the physical variables $[P, T, C]$, where P is the pressure, T the temperature and C , the physical variables target, the CO_2 concentration.

The simulated training data had features with non-Gaussian likelihoods, causing potential problems for spatial learning with Gaussian Processes. While the use of a Variational Gaussian Process helps overcome this issue, we further generalised our training data through the use of a Masked Autoregressive Flow model that transforms the likelihoods of the input features to the family of Gaussian-distributions.

The results of the optimal sensor placement are discussed in the following. Firstly, the scalability issues related to dense grid initialisations of set S are addressed. Secondly, the introduction of the MCMC based fine-tuning algorithm is motivated. Finally, the optimal sensor placement solutions provided by our proposed VGPosp model are presented.

435 The placement Algorithm 2 is executed on a predefined area of interest, in which a
 436 density parameter specifies the grid initialisation that defines set S . Figure 9 demon-
 437 strates the internal state, i.e. mutual information parameter, of the placement algo-
 438 rithm before making a selection. For each coordinate δ_i is computed (Algorithm 2)
 439 and the most optimal coordinate is selected into the final selection set $\mathcal{A}$. For exam-
 440 ple, in Figure 9a, the first sensor will be chosen to be located where δ_i is the highest,
 441 i.e. yellow colour part. From Figure 9, it can be seen that the scale of δ_i is not
 442 the same in each sub-figures and becomes narrower. Indeed, the contributions made
 443 by earlier selections are higher, explaining why the δ_i quantities decrease after more
 444 sensors are added to set S .

445 The running-times shown in Figure 10 are descriptive of the exponential computa-
 446 tional cost that is incurred from selecting a larger input set of S . However, it cannot
 447 be expected from the selection Algorithm 1 to find the optimal locations in contin-
 448 uous space when defining only distant, discrete points. In order to reduce the time
 449 complexity of discovering optimal coordinates in continuous space, we proposed an
 450 MCMC-based fine-tuning method of set S . The impact of this procedure is demon-
 451 strated by Figure 11, where the percentage increase in the optimisation criterion,
 452 mutual information parameter can be multiple orders of magnitude larger than that
 453 of the uniform grid instantiation, which may miss more optimal regions. For example
 454 in the case of a $7 \times 7 \times 1$ grid instantiation, the fine-tuning Algorithm 1 can achieve a
 455 3 order of magnitude improvement in the overall mutual information, associated with
 456 our final selection set $\mathcal{A}$. This improvement is achieved after 15 grid optimisation
 457 attempts. In Figure 12, a $6 \times 6 \times 4$ grid is considered associated with 40 grid opti-
 458 misation attempts for each selection. The optimal selection of 7 sensors are plotted
 459 with crosses as well as all modified grid positions that had achieved improved mutual
 460 information parameter values. Their colour corresponds with the mutual informa-
 461 tion parameter that the coordinate had achieved. The final optimal coordinates of
 462 the room are depicted in Figure 13.

463 Data Assimilation technology is coupled with the predictive model Fluidity. Data
 464 Assimilation uses observed data from sensors to improve and correct the numeri-
 465 cal results from the simulation. 7 sensors are assimilated in the predictive model.
 466 The DA algorithm and methodology used was previously successfully coupled with
 467 Fluidity and is presented in details in [2, 42]. The accuracy of the DA results are
 468 evaluating using the mean squared error: $MSE(C) = \frac{\|C - C^{v,n}\|_{L^2}^2}{\|C^{v,n}\|_{L^2}^2}$, where C is either
 469 C^n the Fluidity concentration at time step n or C^{DA} the corrected concentration
 470 using DA and $C^{v,n}$ is the control variable, i.e. the true observed data. The MSE
 471 is computed using the 7 optimal sensor locations shown in Figure 13 and compared

FIGURE 9. Mutual Information parameter δ_i on M grid points ($11 \times 11 \times 1$) for $k = 7$ sensors. The colours show the value of δ_i and the scale is different on each sub-figures. Yellow and violet colours denote high and low δ_i values respectively.

FIGURE 10. Execution time t of Algorithm 1 as a function of the number of initial grid points M . The y -axis is logarithmic.

FIGURE 11. Percentage increase in mutual information parameter after the fine-tuning Algorithm 1.

FIGURE 12. Fine-tuning of grid-points and final selection coordinates. Colour represents mutual information parameter of placement. The colour of the point shows the value of the Mutual Information. The crosses depict the final optimal sensor locations.

472 with the MSE obtained using 7 sensors located randomly. 2000 random sensors
 473 positioning were performed. Assimilating the seven optimally positioned sensors,
 474 the error of the predictive model, i.e. Fluidity, is reduced by up to three order of
 475 magnitude: $MSE(C^n) = 0.17$ and $MSE(C^{DA}) = 0.0005$. Moreover, this error is

FIGURE 13. Optimal final location of seven sensors in the room of Clarence Centre obtained using the Variational Gaussian Process optimal sensor placement VGPosp in Algorithm 1.

up to two order of magnitude lower than the ones computed using random sensors placement. In one of the worst random case scenario: $MSE(C^{DA}) = 0.023$.

5. CONCLUSION

This work described a novel pipeline for sensor placement, incorporating a Masked Autoregressive Flows (MAF) [20] for preconditioning, a Variational Gaussian Process (VGP) [14, 15] spatial model and a mutual information-based placement algorithm [5]. In this paper, the alterations to the existing placement pipelines are significant as they introduce multiple layers of approximations in order to reduce time complexities. More specifically, VGP was introduced for the sensor placement pipeline to tackle the $O(N^3)$ complexity associated with traditional GP for spatial modelling. Increased model generalisation was achieved with MAF that learn non-linear invertible transformations between complicated transformations and the more flexible Normal distribution. All models and algorithms were implemented as a TensorFlow computational graph to further reduce run-times as opportunities for parallel computation are automatically recognised by the graph compiler. Furthermore, this work proposed and developed two extension algorithms. One focused on incorporating information and sampling environmental features from the time-series for computing mutual information. Secondly, a wrapper algorithm was built to iteratively subsampling and globally optimise the instantiated set of base grid-coordinates, leading to a three-fold increase in mutual information associated with the final selection. The combination of these two algorithms achieved stability and a global improvement in the selection coordinates.

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605 ACCRONYMS

- 606 **CFD:** Computational Fluid Dynamics
- 607 **DA:** Data Assimilation
- 608 **ELBO:** Evidence Lower BOUND
- 609 **GP:** Gaussian Process
- 610 **IAQ:** Indoor Air Quality
- 611 **KL:** Kullback-Leibler
- 612 **LES:** Large Eddy Simulation
- 613 **LSBU:** London South Bank University
- 614 **MADE:** Masked Autoencoder for Distribution Estimation
- 615 **MAF:** Masked Autoregressive Flows
- 616 **MCMC:** Markov-Chain Monte Carlo
- 617 **MI:** Mutual Information
- 618 **SGP:** Sparse Variational Process
- 619 **VGP:** Variational Gaussian Process
- 620 **VGPosp:** Variational Gaussian Process optimal sensor placement

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